



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 01:12 pm GMT

PDB ID : 7AZG
Title : DNA polymerase sliding clamp from Escherichia coli with peptide 4 bound
Authors : Monsarrat, C.; Compain, G.; Andre, C.; Martiel, I.; Engilberge, S.; Olieric, V.;
Wolff, P.; Brillet, K.; Landolfo, M.; Silva da Veiga, C.; Wagner, J.; Guichard,
G.; Burnouf, D.Y.
Deposited on : 2020-11-16
Resolution : 2.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

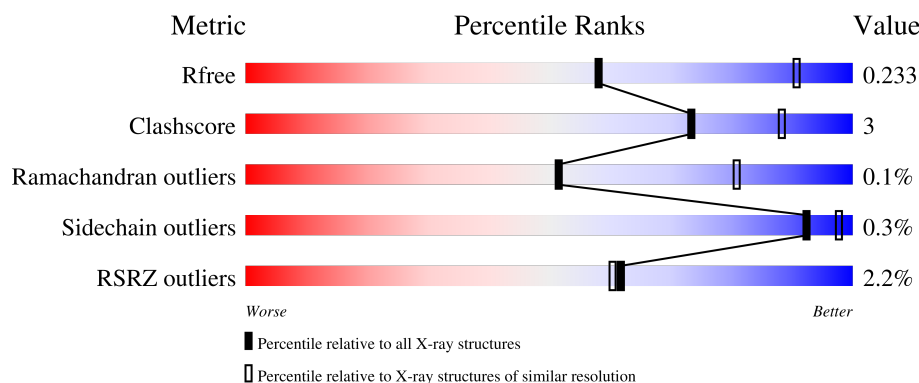
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	
1	B	386	
1	C	386	
1	D	386	
1	E	386	

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Mol	Chain	Length	Quality of chain
1	F	386	 % 84% 11% 5%
1	G	386	 6% 87% 7% 6%
1	H	386	 5% 90% 6% 5%
2	I	6	 83% 17%
2	J	6	 67% 33%
2	K	6	 83% 17%
2	L	6	 50% 50%
2	M	6	 67% 33%
2	N	6	 83% 17%
2	O	6	 83% 17%
2	P	6	 83% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23648 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	4	0
			2878	1809	507	543	19			
1	B	368	Total	C	N	O	S	0	1	0
			2865	1801	502	543	19			
1	C	368	Total	C	N	O	S	0	2	0
			2866	1800	507	540	19			
1	D	368	Total	C	N	O	S	0	2	0
			2864	1796	505	544	19			
1	E	368	Total	C	N	O	S	0	0	0
			2848	1788	499	542	19			
1	F	367	Total	C	N	O	S	0	1	0
			2837	1784	495	539	19			
1	G	362	Total	C	N	O	S	0	0	0
			2781	1750	488	524	19			
1	H	368	Total	C	N	O	S	0	0	0
			2788	1751	485	534	18			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A073FMV0
A	-18	GLY	-	expression tag	UNP A0A073FMV0
A	-17	SER	-	expression tag	UNP A0A073FMV0
A	-16	SER	-	expression tag	UNP A0A073FMV0
A	-15	HIS	-	expression tag	UNP A0A073FMV0
A	-14	HIS	-	expression tag	UNP A0A073FMV0
A	-13	HIS	-	expression tag	UNP A0A073FMV0
A	-12	HIS	-	expression tag	UNP A0A073FMV0
A	-11	HIS	-	expression tag	UNP A0A073FMV0
A	-10	HIS	-	expression tag	UNP A0A073FMV0
A	-9	SER	-	expression tag	UNP A0A073FMV0
A	-8	SER	-	expression tag	UNP A0A073FMV0
A	-7	GLY	-	expression tag	UNP A0A073FMV0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP A0A073FMV0
A	-5	VAL	-	expression tag	UNP A0A073FMV0
A	-4	PRO	-	expression tag	UNP A0A073FMV0
A	-3	ARG	-	expression tag	UNP A0A073FMV0
A	-2	GLY	-	expression tag	UNP A0A073FMV0
A	-1	SER	-	expression tag	UNP A0A073FMV0
A	0	HIS	-	expression tag	UNP A0A073FMV0
B	-19	MET	-	initiating methionine	UNP A0A073FMV0
B	-18	GLY	-	expression tag	UNP A0A073FMV0
B	-17	SER	-	expression tag	UNP A0A073FMV0
B	-16	SER	-	expression tag	UNP A0A073FMV0
B	-15	HIS	-	expression tag	UNP A0A073FMV0
B	-14	HIS	-	expression tag	UNP A0A073FMV0
B	-13	HIS	-	expression tag	UNP A0A073FMV0
B	-12	HIS	-	expression tag	UNP A0A073FMV0
B	-11	HIS	-	expression tag	UNP A0A073FMV0
B	-10	HIS	-	expression tag	UNP A0A073FMV0
B	-9	SER	-	expression tag	UNP A0A073FMV0
B	-8	SER	-	expression tag	UNP A0A073FMV0
B	-7	GLY	-	expression tag	UNP A0A073FMV0
B	-6	LEU	-	expression tag	UNP A0A073FMV0
B	-5	VAL	-	expression tag	UNP A0A073FMV0
B	-4	PRO	-	expression tag	UNP A0A073FMV0
B	-3	ARG	-	expression tag	UNP A0A073FMV0
B	-2	GLY	-	expression tag	UNP A0A073FMV0
B	-1	SER	-	expression tag	UNP A0A073FMV0
B	0	HIS	-	expression tag	UNP A0A073FMV0
C	-19	MET	-	initiating methionine	UNP A0A073FMV0
C	-18	GLY	-	expression tag	UNP A0A073FMV0
C	-17	SER	-	expression tag	UNP A0A073FMV0
C	-16	SER	-	expression tag	UNP A0A073FMV0
C	-15	HIS	-	expression tag	UNP A0A073FMV0
C	-14	HIS	-	expression tag	UNP A0A073FMV0
C	-13	HIS	-	expression tag	UNP A0A073FMV0
C	-12	HIS	-	expression tag	UNP A0A073FMV0
C	-11	HIS	-	expression tag	UNP A0A073FMV0
C	-10	HIS	-	expression tag	UNP A0A073FMV0
C	-9	SER	-	expression tag	UNP A0A073FMV0
C	-8	SER	-	expression tag	UNP A0A073FMV0
C	-7	GLY	-	expression tag	UNP A0A073FMV0
C	-6	LEU	-	expression tag	UNP A0A073FMV0
C	-5	VAL	-	expression tag	UNP A0A073FMV0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP A0A073FMV0
C	-3	ARG	-	expression tag	UNP A0A073FMV0
C	-2	GLY	-	expression tag	UNP A0A073FMV0
C	-1	SER	-	expression tag	UNP A0A073FMV0
C	0	HIS	-	expression tag	UNP A0A073FMV0
D	-19	MET	-	initiating methionine	UNP A0A073FMV0
D	-18	GLY	-	expression tag	UNP A0A073FMV0
D	-17	SER	-	expression tag	UNP A0A073FMV0
D	-16	SER	-	expression tag	UNP A0A073FMV0
D	-15	HIS	-	expression tag	UNP A0A073FMV0
D	-14	HIS	-	expression tag	UNP A0A073FMV0
D	-13	HIS	-	expression tag	UNP A0A073FMV0
D	-12	HIS	-	expression tag	UNP A0A073FMV0
D	-11	HIS	-	expression tag	UNP A0A073FMV0
D	-10	HIS	-	expression tag	UNP A0A073FMV0
D	-9	SER	-	expression tag	UNP A0A073FMV0
D	-8	SER	-	expression tag	UNP A0A073FMV0
D	-7	GLY	-	expression tag	UNP A0A073FMV0
D	-6	LEU	-	expression tag	UNP A0A073FMV0
D	-5	VAL	-	expression tag	UNP A0A073FMV0
D	-4	PRO	-	expression tag	UNP A0A073FMV0
D	-3	ARG	-	expression tag	UNP A0A073FMV0
D	-2	GLY	-	expression tag	UNP A0A073FMV0
D	-1	SER	-	expression tag	UNP A0A073FMV0
D	0	HIS	-	expression tag	UNP A0A073FMV0
E	-19	MET	-	initiating methionine	UNP A0A073FMV0
E	-18	GLY	-	expression tag	UNP A0A073FMV0
E	-17	SER	-	expression tag	UNP A0A073FMV0
E	-16	SER	-	expression tag	UNP A0A073FMV0
E	-15	HIS	-	expression tag	UNP A0A073FMV0
E	-14	HIS	-	expression tag	UNP A0A073FMV0
E	-13	HIS	-	expression tag	UNP A0A073FMV0
E	-12	HIS	-	expression tag	UNP A0A073FMV0
E	-11	HIS	-	expression tag	UNP A0A073FMV0
E	-10	HIS	-	expression tag	UNP A0A073FMV0
E	-9	SER	-	expression tag	UNP A0A073FMV0
E	-8	SER	-	expression tag	UNP A0A073FMV0
E	-7	GLY	-	expression tag	UNP A0A073FMV0
E	-6	LEU	-	expression tag	UNP A0A073FMV0
E	-5	VAL	-	expression tag	UNP A0A073FMV0
E	-4	PRO	-	expression tag	UNP A0A073FMV0
E	-3	ARG	-	expression tag	UNP A0A073FMV0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP A0A073FMV0
E	-1	SER	-	expression tag	UNP A0A073FMV0
E	0	HIS	-	expression tag	UNP A0A073FMV0
F	-19	MET	-	initiating methionine	UNP A0A073FMV0
F	-18	GLY	-	expression tag	UNP A0A073FMV0
F	-17	SER	-	expression tag	UNP A0A073FMV0
F	-16	SER	-	expression tag	UNP A0A073FMV0
F	-15	HIS	-	expression tag	UNP A0A073FMV0
F	-14	HIS	-	expression tag	UNP A0A073FMV0
F	-13	HIS	-	expression tag	UNP A0A073FMV0
F	-12	HIS	-	expression tag	UNP A0A073FMV0
F	-11	HIS	-	expression tag	UNP A0A073FMV0
F	-10	HIS	-	expression tag	UNP A0A073FMV0
F	-9	SER	-	expression tag	UNP A0A073FMV0
F	-8	SER	-	expression tag	UNP A0A073FMV0
F	-7	GLY	-	expression tag	UNP A0A073FMV0
F	-6	LEU	-	expression tag	UNP A0A073FMV0
F	-5	VAL	-	expression tag	UNP A0A073FMV0
F	-4	PRO	-	expression tag	UNP A0A073FMV0
F	-3	ARG	-	expression tag	UNP A0A073FMV0
F	-2	GLY	-	expression tag	UNP A0A073FMV0
F	-1	SER	-	expression tag	UNP A0A073FMV0
F	0	HIS	-	expression tag	UNP A0A073FMV0
G	-19	MET	-	initiating methionine	UNP A0A073FMV0
G	-18	GLY	-	expression tag	UNP A0A073FMV0
G	-17	SER	-	expression tag	UNP A0A073FMV0
G	-16	SER	-	expression tag	UNP A0A073FMV0
G	-15	HIS	-	expression tag	UNP A0A073FMV0
G	-14	HIS	-	expression tag	UNP A0A073FMV0
G	-13	HIS	-	expression tag	UNP A0A073FMV0
G	-12	HIS	-	expression tag	UNP A0A073FMV0
G	-11	HIS	-	expression tag	UNP A0A073FMV0
G	-10	HIS	-	expression tag	UNP A0A073FMV0
G	-9	SER	-	expression tag	UNP A0A073FMV0
G	-8	SER	-	expression tag	UNP A0A073FMV0
G	-7	GLY	-	expression tag	UNP A0A073FMV0
G	-6	LEU	-	expression tag	UNP A0A073FMV0
G	-5	VAL	-	expression tag	UNP A0A073FMV0
G	-4	PRO	-	expression tag	UNP A0A073FMV0
G	-3	ARG	-	expression tag	UNP A0A073FMV0
G	-2	GLY	-	expression tag	UNP A0A073FMV0
G	-1	SER	-	expression tag	UNP A0A073FMV0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A073FMV0
H	-19	MET	-	initiating methionine	UNP A0A073FMV0
H	-18	GLY	-	expression tag	UNP A0A073FMV0
H	-17	SER	-	expression tag	UNP A0A073FMV0
H	-16	SER	-	expression tag	UNP A0A073FMV0
H	-15	HIS	-	expression tag	UNP A0A073FMV0
H	-14	HIS	-	expression tag	UNP A0A073FMV0
H	-13	HIS	-	expression tag	UNP A0A073FMV0
H	-12	HIS	-	expression tag	UNP A0A073FMV0
H	-11	HIS	-	expression tag	UNP A0A073FMV0
H	-10	HIS	-	expression tag	UNP A0A073FMV0
H	-9	SER	-	expression tag	UNP A0A073FMV0
H	-8	SER	-	expression tag	UNP A0A073FMV0
H	-7	GLY	-	expression tag	UNP A0A073FMV0
H	-6	LEU	-	expression tag	UNP A0A073FMV0
H	-5	VAL	-	expression tag	UNP A0A073FMV0
H	-4	PRO	-	expression tag	UNP A0A073FMV0
H	-3	ARG	-	expression tag	UNP A0A073FMV0
H	-2	GLY	-	expression tag	UNP A0A073FMV0
H	-1	SER	-	expression tag	UNP A0A073FMV0
H	0	HIS	-	expression tag	UNP A0A073FMV0

- Molecule 2 is a protein called Peptide 4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	0
			52	36	6	10			
2	J	6	Total	C	N	O	0	0	0
			52	36	6	10			
2	K	6	Total	C	N	O	0	0	0
			52	36	6	10			
2	L	6	Total	C	N	O	0	0	0
			52	36	6	10			
2	M	6	Total	C	N	O	0	0	0
			52	36	6	10			
2	N	6	Total	C	N	O	0	0	0
			52	36	6	10			
2	O	6	Total	C	N	O	0	0	0
			52	36	6	10			
2	P	6	Total	C	N	O	0	0	0
			52	36	6	10			

- Molecule 3 is water.

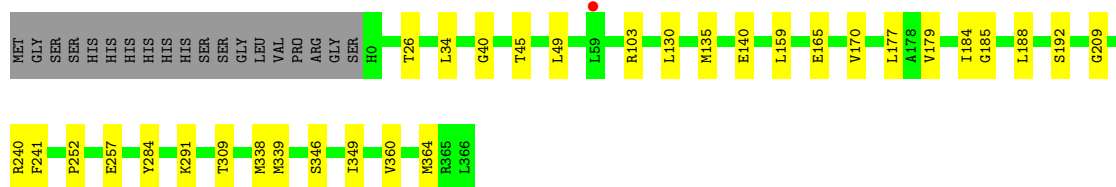
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total 84	O 84	0	0
3	B	58	Total 58	O 58	0	0
3	C	79	Total 79	O 79	0	0
3	D	70	Total 71	O 71	0	1
3	E	68	Total 68	O 68	0	0
3	F	49	Total 49	O 49	0	0
3	G	55	Total 55	O 55	0	0
3	H	35	Total 35	O 35	0	0
3	I	1	Total 1	O 1	0	0
3	J	1	Total 1	O 1	0	0
3	K	1	Total 1	O 1	0	0
3	L	1	Total 1	O 1	0	0
3	O	1	Total 1	O 1	0	0
3	P	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

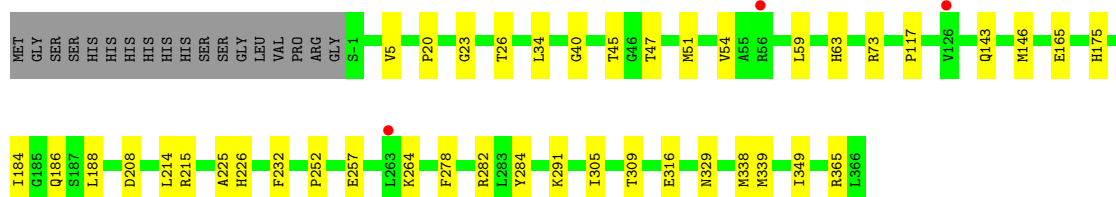
- Molecule 1: Beta sliding clamp

Chain A: 



- Molecule 1: Beta sliding clamp

Chain B: 




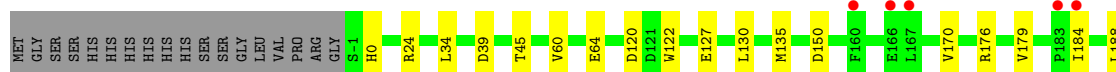
- Molecule 1: Beta sliding clamp

Chain C: 



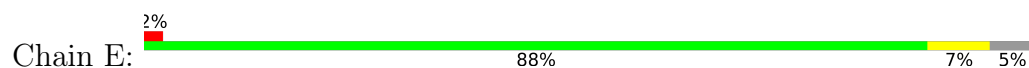
- Molecule 1: Beta sliding clamp

Chain D: 

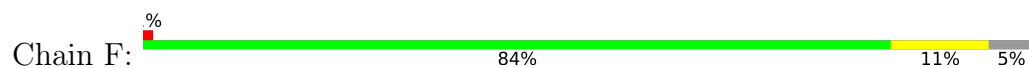




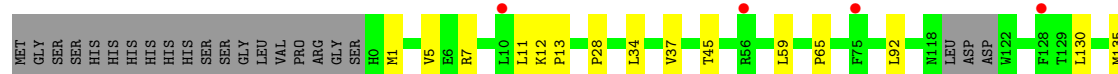
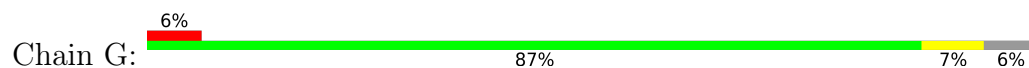
- Molecule 1: Beta sliding clamp



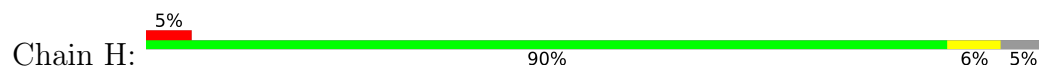
- Molecule 1: Beta sliding clamp



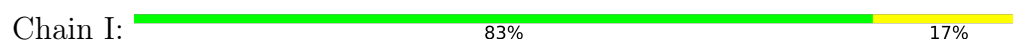
- Molecule 1: Beta sliding clamp



- Molecule 1: Beta sliding clamp



- Molecule 2: Peptide 4

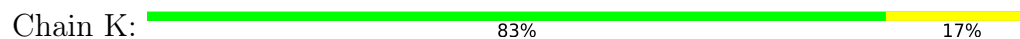




- Molecule 2: Peptide 4



- Molecule 2: Peptide 4



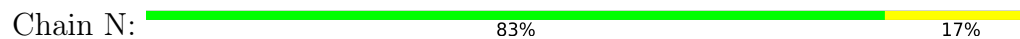
- Molecule 2: Peptide 4



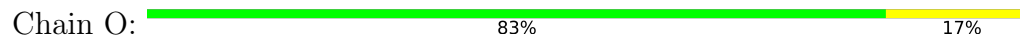
- Molecule 2: Peptide 4



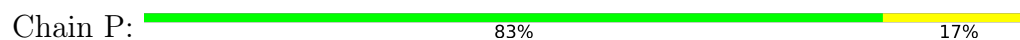
- Molecule 2: Peptide 4



- Molecule 2: Peptide 4



- Molecule 2: Peptide 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.42Å 165.30Å 138.51Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	33.65 – 2.92 106.13 – 2.92	Depositor EDS
% Data completeness (in resolution range)	68.6 (33.65-2.92) 68.6 (106.13-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.184 , 0.234 0.189 , 0.233	Depositor DCC
R_{free} test set	2290 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23648	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SOQ, ALC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2942	0.52	0/3981
1	B	0.39	0/2919	0.52	0/3951
1	C	0.38	0/2922	0.49	0/3954
1	D	0.39	0/2920	0.53	0/3954
1	E	0.36	0/2898	0.49	0/3924
1	F	0.36	0/2891	0.51	0/3917
1	G	0.35	0/2828	0.50	0/3827
1	H	0.32	0/2838	0.48	0/3853
2	I	0.48	0/31	0.54	0/37
2	J	0.56	0/31	0.59	0/37
2	K	0.47	0/31	0.60	0/37
2	L	0.45	0/31	0.59	0/37
2	M	0.45	0/31	0.62	0/37
2	N	0.43	0/31	0.47	0/37
2	O	0.42	0/31	0.43	0/37
2	P	0.47	0/31	0.48	0/37
All	All	0.37	0/23406	0.51	0/31657

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2878	0	2897	16	0
1	B	2865	0	2878	26	0
1	C	2866	0	2884	10	0
1	D	2864	0	2866	24	0
1	E	2848	0	2850	19	0
1	F	2837	0	2832	31	0
1	G	2781	0	2787	16	0
1	H	2788	0	2734	13	0
2	I	52	0	42	1	0
2	J	52	0	42	3	0
2	K	52	0	42	1	0
2	L	52	0	42	4	0
2	M	52	0	42	3	0
2	N	52	0	42	1	0
2	O	52	0	42	1	0
2	P	52	0	42	0	0
3	A	84	0	0	0	0
3	B	58	0	0	2	0
3	C	79	0	0	0	0
3	D	71	0	0	0	0
3	E	68	0	0	0	0
3	F	49	0	0	0	0
3	G	55	0	0	0	0
3	H	35	0	0	1	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
All	All	23648	0	23064	150	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:LEU:HD13	1:F:333:CYS:SG	2.16	0.85
1:G:344:VAL:HG13	2:O:3:ALC:HE12	1.61	0.82
1:B:47:THR:HG21	1:B:117:PRO:HG2	1.66	0.77
1:D:331:LEU:HD13	1:D:333:CYS:SG	2.27	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:LEU:HD12	1:D:331:LEU:O	1.89	0.73
1:E:364:MET:HB3	2:M:2:GLN:HA	1.73	0.70
1:F:214:LEU:HD13	1:F:227:VAL:HG22	1.74	0.69
1:B:252:PRO:HB2	1:B:339:MET:HB3	1.75	0.69
1:F:331:LEU:HD12	1:F:331:LEU:O	1.93	0.69
1:E:214:LEU:HD13	1:E:227:VAL:HG22	1.73	0.68
1:E:184:ILE:HD11	1:E:188:LEU:HD11	1.77	0.67
1:H:184:ILE:HD11	1:H:188:LEU:HD11	1.77	0.67
1:B:365:ARG:HB2	2:J:3:ALC:HZ3	1.77	0.66
1:A:184:ILE:HD11	1:A:188:LEU:HD11	1.78	0.65
1:B:264:LYS:HD2	1:B:329:ASN:OD1	1.95	0.65
1:C:184:ILE:HD11	1:C:188:LEU:HD11	1.79	0.64
1:B:26:THR:HA	1:C:28:PRO:HG2	1.80	0.63
1:B:184:ILE:HD11	1:B:188:LEU:HD11	1.79	0.63
1:F:184:ILE:HD11	1:F:188:LEU:HD11	1.79	0.62
1:E:365:ARG:HB2	2:M:3:ALC:HZ3	1.80	0.62
1:E:148:HIS:ND1	1:E:149:GLN:HG2	2.15	0.61
1:B:40:GLY:HA2	1:B:63:HIS:NE2	2.16	0.61
1:A:240:ARG:NH1	1:A:241:PHE:O	2.34	0.60
1:E:26:THR:O	1:H:24:ARG:CB	2.50	0.60
1:H:96:ARG:NE	1:H:107:SER:OG	2.35	0.59
1:C:285:VAL:CG2	1:C:315:MET:HG2	2.34	0.58
1:F:331:LEU:HD11	1:F:336:VAL:CG1	2.34	0.57
1:F:1:MET:CE	1:F:68:THR:HG22	2.34	0.57
1:E:283:LEU:HG	1:E:290:LEU:HD11	1.86	0.56
1:B:51:MET:HE3	1:B:232:PHE:HE1	1.70	0.56
1:B:54:VAL:HG23	3:B:409:HOH:O	2.06	0.56
1:D:365:ARG:HB2	2:L:3:ALC:HZ3	1.88	0.56
1:E:168:ARG:HG3	1:E:181:SER:HB3	1.88	0.56
1:D:184:ILE:HD11	1:D:188:LEU:HD11	1.88	0.56
1:G:344:VAL:HG12	1:G:344:VAL:O	2.06	0.56
1:F:165:GLU:HA	1:F:186:GLN:O	2.06	0.55
1:F:214:LEU:HD13	1:F:227:VAL:CG2	2.36	0.55
1:D:170:VAL:HG22	1:D:179:VAL:HG23	1.89	0.55
1:B:278:PHE:CE2	1:D:150:ASP:HA	2.42	0.54
1:F:331:LEU:CD1	1:F:333:CYS:SG	2.93	0.53
1:D:0:HIS:HB2	1:D:64:GLU:OE1	2.08	0.53
1:G:37:VAL:HG13	1:G:65:PRO:HA	1.90	0.52
1:E:28:PRO:HG2	1:H:26:THR:HA	1.91	0.52
1:F:176:ARG:NH1	1:F:326:ASP:OD2	2.43	0.52
1:H:135:MET:HB3	1:H:207:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:PRO:O	2:M:3:ALC:HB3	2.09	0.51
1:C:165:GLU:HA	1:C:186:GLN:O	2.11	0.50
1:C:6:GLU:HB3	1:C:9:HIS:CE1	2.46	0.50
1:E:161:GLU:OE2	1:E:168:ARG:NH1	2.45	0.50
1:D:331:LEU:HD11	1:D:336:VAL:CG1	2.42	0.50
1:D:331:LEU:CD1	1:D:333:CYS:SG	2.98	0.49
1:E:42:LEU:HB2	1:E:59:LEU:HD11	1.94	0.49
1:D:247:VAL:HG13	2:L:5:LEU:HD22	1.94	0.49
1:A:364:MET:HB3	2:I:2:GLN:HA	1.94	0.49
1:F:214:LEU:CD1	1:F:227:VAL:HG22	2.42	0.48
1:B:284:TYR:HB2	1:B:291:LYS:HB3	1.95	0.48
1:F:1:MET:HE1	1:F:68:THR:HG22	1.96	0.47
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.95	0.47
1:B:215:ARG:HB3	1:B:226:HIS:HB2	1.97	0.47
1:D:127:GLU:HG2	1:D:215:ARG:HE	1.79	0.47
1:G:214:LEU:HD11	1:G:225:ALA:HB1	1.96	0.47
1:F:331:LEU:HD11	1:F:336:VAL:HG12	1.95	0.47
1:B:143:GLN:O	1:B:146:MET:HE2	2.15	0.47
1:B:34:LEU:HB3	1:B:45:THR:HB	1.97	0.47
1:B:175:HIS:CE1	2:J:2:GLN:HG2	2.50	0.47
1:G:5:VAL:HG22	1:G:59:LEU:HD13	1.97	0.47
1:H:284:TYR:HB2	1:H:291:LYS:HB3	1.97	0.47
1:A:284:TYR:HB2	1:A:291:LYS:HB3	1.98	0.46
1:B:143:GLN:HA	1:B:146:MET:HE2	1.97	0.46
1:C:284:TYR:HB2	1:C:291:LYS:HB3	1.97	0.46
1:H:203:LEU:HD12	1:H:206:MET:HE2	1.98	0.46
1:F:284:TYR:HB2	1:F:291:LYS:HB3	1.97	0.46
1:D:284:TYR:HB2	1:D:291:LYS:HB3	1.98	0.46
1:G:284:TYR:HB2	1:G:291:LYS:HB3	1.97	0.46
1:F:189:PRO:HB2	1:F:191[B]:HIS:CE1	2.52	0.45
1:A:159:LEU:HD11	1:A:192:SER:OG	2.16	0.45
1:E:214:LEU:HD13	1:E:227:VAL:CG2	2.44	0.45
1:A:130:LEU:HD11	1:A:135:MET:HB2	1.99	0.45
1:C:214:LEU:HD11	1:C:225:ALA:HB1	1.98	0.45
1:F:26:THR:HA	1:G:28:PRO:HG2	1.98	0.45
1:G:7:ARG:CZ	1:G:11:LEU:HD11	2.47	0.45
1:B:165:GLU:HA	1:B:186:GLN:O	2.17	0.45
1:F:1:MET:HE2	1:F:68:THR:HG22	1.99	0.45
1:F:159:LEU:O	1:F:169:THR:HA	2.17	0.44
1:A:346:SER:HB3	1:A:360:VAL:HG13	1.99	0.44
1:A:103:ARG:HB3	1:B:305:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:VAL:CG2	2:L:6:PHE:HE1	2.31	0.44
1:F:278:PHE:CE2	1:H:150:ASP:HA	2.53	0.44
1:H:214:LEU:HD11	1:H:225:ALA:HB1	1.99	0.44
1:E:130:LEU:HD11	1:E:135:MET:HB2	2.00	0.44
1:E:257:GLU:HB2	1:E:309:THR:HB	2.00	0.44
1:A:165:GLU:OE2	1:A:185:GLY:HA2	2.18	0.44
1:A:177:LEU:HB3	1:A:360:VAL:HB	1.98	0.44
1:B:282:ARG:HD3	1:B:316:GLU:OE2	2.18	0.44
1:D:39:ASP:HB3	1:F:191[B]:HIS:HD2	1.83	0.44
1:A:252:PRO:HG2	1:A:339:MET:HB3	2.00	0.43
1:G:1:MET:HB3	1:G:92:LEU:HD12	1.99	0.43
1:H:16:GLN:HG3	1:H:230:PHE:CZ	2.53	0.43
1:F:34:LEU:HB3	1:F:45:THR:HB	2.01	0.43
1:G:315:MET:SD	1:G:340:LEU:HD23	2.57	0.43
1:D:338:MET:HG2	1:D:349:ILE:HG12	2.01	0.43
1:F:214:LEU:HD11	1:F:225:ALA:HB1	1.99	0.43
1:F:282:ARG:HG2	1:F:366:LEU:HD23	1.99	0.43
1:D:130:LEU:HD11	1:D:135:MET:HB2	1.99	0.43
1:D:214:LEU:HD11	1:D:225:ALA:HB1	2.00	0.43
1:A:34:LEU:HB3	1:A:45:THR:HB	2.01	0.43
1:E:214:LEU:HD11	1:E:225:ALA:HB1	2.01	0.43
1:G:130:LEU:HD11	1:G:135:MET:HB2	2.01	0.42
1:D:34:LEU:HB3	1:D:45:THR:HB	2.00	0.42
1:H:130:LEU:HD11	1:H:135:MET:HB2	2.00	0.42
1:G:257:GLU:HB2	1:G:309:THR:HB	2.01	0.42
1:A:257:GLU:HB2	1:A:309:THR:HB	2.02	0.42
1:E:214:LEU:CD1	1:E:227:VAL:HG22	2.45	0.42
1:E:27:LEU:HB2	1:E:30:LEU:HG	2.02	0.42
1:A:26:THR:OG1	1:D:24:ARG:HG3	2.20	0.42
1:H:34:LEU:HB3	1:H:45:THR:HB	2.01	0.42
1:F:130:LEU:HD11	1:F:135:MET:HB2	2.01	0.42
1:G:344:VAL:O	1:G:344:VAL:CG1	2.67	0.42
1:H:59:LEU:HB3	3:H:406:HOH:O	2.20	0.42
1:C:21:LEU:CD1	1:C:21:LEU:N	2.83	0.42
1:F:257:GLU:HB2	1:F:309:THR:HB	2.02	0.42
1:A:338:MET:HG2	1:A:349:ILE:HG12	2.01	0.41
1:B:20:PRO:HB3	1:B:51:MET:HE1	2.01	0.41
1:F:338:MET:HG2	1:F:349:ILE:HG12	2.01	0.41
1:D:176:ARG:NH1	1:D:326:ASP:OD2	2.53	0.41
1:A:170:VAL:HG22	1:A:179:VAL:HG23	2.01	0.41
1:B:252:PRO:CB	1:B:339:MET:HB3	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:LEU:C	1:F:13:PRO:HD2	2.40	0.41
1:F:252:PRO:HA	1:F:341:THR:HG22	2.01	0.41
1:G:34:LEU:HB3	1:G:45:THR:HB	2.01	0.41
1:B:338:MET:HG2	1:B:349:ILE:HG12	2.02	0.41
1:E:338:MET:HG2	1:E:349:ILE:HG12	2.02	0.41
1:D:120:ASP:O	1:D:122:TRP:HD1	2.03	0.41
2:L:3:ALC:HD22	2:L:3:ALC:HA	1.92	0.41
1:G:338:MET:HG2	1:G:349:ILE:HG12	2.01	0.41
2:K:3:ALC:HD22	2:K:3:ALC:HA	1.93	0.41
1:B:257:GLU:HB2	1:B:309:THR:HB	2.03	0.41
1:D:257:GLU:HB2	1:D:309:THR:HB	2.02	0.41
1:C:250:LYS:HA	1:C:250:LYS:HD3	1.92	0.40
1:B:5:VAL:HG22	1:B:59:LEU:HD23	2.03	0.40
1:F:122:TRP:HZ2	1:F:224:ARG:HB2	1.86	0.40
2:J:3:ALC:HD22	2:J:3:ALC:HA	1.97	0.40
2:N:3:ALC:HD22	2:N:3:ALC:HA	1.90	0.40
1:B:73:ARG:NH2	3:B:402:HOH:O	2.52	0.40
1:C:130:LEU:HD11	1:C:135:MET:HB2	2.03	0.40
1:D:320:ASN:HB3	1:D:323:TYR:CD2	2.57	0.40
1:G:12:LYS:N	1:G:13:PRO:HD2	2.36	0.40
1:D:127:GLU:HG3	1:D:217:GLN:HG2	2.03	0.40
1:F:132:GLN:HG3	1:F:212:ASN:O	2.22	0.40
1:F:263:LEU:HD23	1:F:328:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	368/386 (95%)	355 (96%)	10 (3%)	3 (1%)	19 49
1	B	367/386 (95%)	355 (97%)	11 (3%)	1 (0%)	41 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	368/386 (95%)	359 (98%)	9 (2%)	0	100	100
1	D	368/386 (95%)	357 (97%)	11 (3%)	0	100	100
1	E	366/386 (95%)	353 (96%)	13 (4%)	0	100	100
1	F	366/386 (95%)	357 (98%)	9 (2%)	0	100	100
1	G	356/386 (92%)	344 (97%)	12 (3%)	0	100	100
1	H	366/386 (95%)	352 (96%)	14 (4%)	0	100	100
2	I	2/6 (33%)	2 (100%)	0	0	100	100
2	J	2/6 (33%)	2 (100%)	0	0	100	100
2	K	2/6 (33%)	2 (100%)	0	0	100	100
2	L	2/6 (33%)	2 (100%)	0	0	100	100
2	M	2/6 (33%)	2 (100%)	0	0	100	100
2	N	2/6 (33%)	2 (100%)	0	0	100	100
2	O	2/6 (33%)	2 (100%)	0	0	100	100
2	P	2/6 (33%)	2 (100%)	0	0	100	100
All	All	2941/3136 (94%)	2848 (97%)	89 (3%)	4 (0%)	51	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLY
1	A	49	LEU
1	A	209	GLY
1	B	23	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/330 (96%)	316 (100%)	1 (0%)	92	98
1	B	315/330 (96%)	314 (100%)	1 (0%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	314/330 (95%)	314 (100%)	0	100	100
1	D	314/330 (95%)	313 (100%)	1 (0%)	92	98
1	E	312/330 (94%)	312 (100%)	0	100	100
1	F	310/330 (94%)	308 (99%)	2 (1%)	86	95
1	G	303/330 (92%)	303 (100%)	0	100	100
1	H	298/330 (90%)	297 (100%)	1 (0%)	92	98
2	I	3/3 (100%)	3 (100%)	0	100	100
2	J	3/3 (100%)	3 (100%)	0	100	100
2	K	3/3 (100%)	3 (100%)	0	100	100
2	L	3/3 (100%)	3 (100%)	0	100	100
2	M	3/3 (100%)	3 (100%)	0	100	100
2	N	3/3 (100%)	3 (100%)	0	100	100
2	O	3/3 (100%)	3 (100%)	0	100	100
2	P	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	2507/2664 (94%)	2500 (100%)	7 (0%)	92	98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	GLU
1	B	208	ASP
1	D	60	VAL
1	F	96	ARG
1	F	286	SER
1	H	41	THR
2	P	6	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	221	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

8 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	367/386 (95%)	-0.42	1 (0%) 94 94	22, 52, 79, 117	0
1	B	368/386 (95%)	-0.27	3 (0%) 86 86	23, 54, 87, 109	0
1	C	368/386 (95%)	-0.29	2 (0%) 91 91	24, 59, 90, 125	0
1	D	368/386 (95%)	-0.16	8 (2%) 62 60	27, 63, 97, 113	0
1	E	368/386 (95%)	-0.19	6 (1%) 72 71	31, 62, 90, 105	0
1	F	367/386 (95%)	-0.12	4 (1%) 80 81	30, 66, 96, 122	0
1	G	362/386 (93%)	0.24	22 (6%) 21 18	48, 88, 117, 163	0
1	H	368/386 (95%)	0.12	19 (5%) 27 24	38, 83, 110, 127	0
2	I	4/6 (66%)	-0.15	0 100 100	31, 32, 44, 44	0
2	J	4/6 (66%)	-0.44	0 100 100	19, 23, 37, 56	0
2	K	4/6 (66%)	-0.51	0 100 100	24, 32, 33, 41	0
2	L	4/6 (66%)	-0.18	0 100 100	31, 34, 53, 59	0
2	M	4/6 (66%)	0.13	0 100 100	37, 56, 56, 60	0
2	N	4/6 (66%)	0.23	0 100 100	52, 55, 61, 68	0
2	O	4/6 (66%)	-0.09	0 100 100	54, 59, 59, 63	0
2	P	4/6 (66%)	0.68	0 100 100	58, 67, 71, 75	0
All	All	2968/3136 (94%)	-0.14	65 (2%) 62 60	19, 65, 104, 163	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	285	VAL	7.9
1	G	160	PHE	6.3
1	G	284	TYR	5.9
1	G	290	LEU	5.8
1	G	283	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	183	PRO	4.5
1	G	190	SER	4.2
1	G	317	ILE	4.1
1	D	285	VAL	4.0
1	H	348	GLN	3.8
1	E	263	LEU	3.8
1	G	167	LEU	3.7
1	G	306	LEU	3.6
1	G	338	MET	3.6
1	G	56	ARG	3.6
1	G	256	LEU	3.4
1	E	340	LEU	3.2
1	G	128	PHE	3.2
1	F	311	SER	3.1
1	H	60	VAL	2.9
1	G	263	LEU	2.9
1	F	128	PHE	2.8
1	D	184	ILE	2.8
1	H	3	PHE	2.8
1	H	108	LEU	2.7
1	H	285	VAL	2.7
1	G	75	PHE	2.7
1	H	37	VAL	2.7
1	E	242	PRO	2.6
1	H	244	TYR	2.6
1	H	317	ILE	2.6
1	G	188	LEU	2.6
1	B	126	VAL	2.5
1	G	292	ILE	2.5
1	C	59	LEU	2.5
1	E	290	LEU	2.5
1	H	360	VAL	2.5
1	B	56	ARG	2.4
1	G	311	SER	2.4
1	G	348	GLN	2.4
1	F	117	PRO	2.4
1	H	344	VAL	2.4
1	C	99	VAL	2.3
1	H	316	GLU	2.3
1	D	160	PHE	2.3
1	D	167	LEU	2.3
1	G	347	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	263	LEU	2.2
1	H	339	MET	2.2
1	E	256	LEU	2.2
1	H	314	GLU	2.2
1	H	59	LEU	2.2
1	E	338	MET	2.1
1	H	49	LEU	2.1
1	H	282	ARG	2.1
1	G	10	LEU	2.1
1	D	166	GLU	2.1
1	D	284	TYR	2.1
1	D	340	LEU	2.1
1	H	203	LEU	2.1
1	H	117	PRO	2.1
1	A	59	LEU	2.1
1	G	267	PHE	2.1
1	F	347	VAL	2.0
1	H	20	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ALC	L	3	11/12	0.96	0.20	37,39,51,53	0
2	ALC	M	3	11/12	0.97	0.16	41,46,56,58	0
2	ALC	N	3	11/12	0.97	0.28	58,67,80,81	0
2	ALC	O	3	11/12	0.97	0.25	55,60,65,65	0
2	ALC	P	3	11/12	0.97	0.23	68,76,79,79	0
2	ALC	K	3	11/12	0.98	0.16	18,25,37,39	0
2	ALC	I	3	11/12	0.98	0.17	23,29,41,41	0
2	ALC	J	3	11/12	0.98	0.16	8,17,31,32	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.